Supplementary Information

Computational predictions on the interactions of parabens with a dipalmitoylphosphatidylcholine lipid bilayer and the human serum albumin protein

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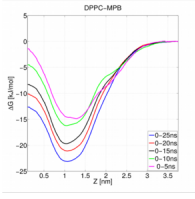
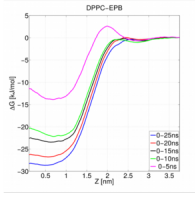
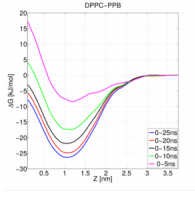
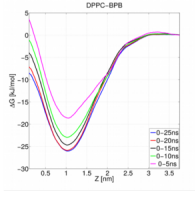
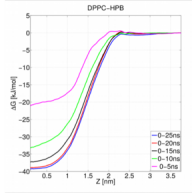
1) PMF simulations convergence criteria:



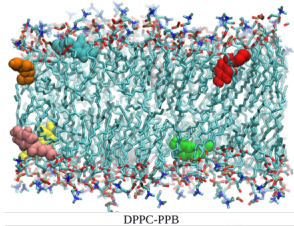




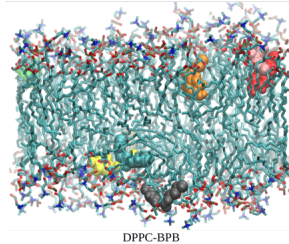




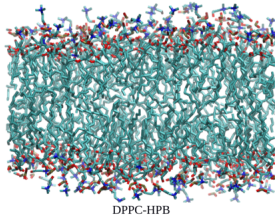
2) Molecular dynamics final snap-shots for paraben adsorption on lipid bilayer surface:



DPPC-PPB



DPPC-BPB



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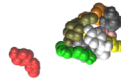
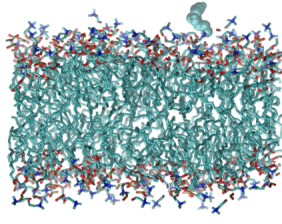
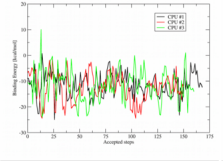
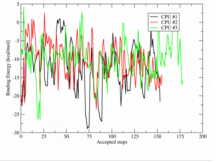


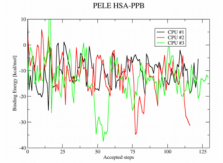


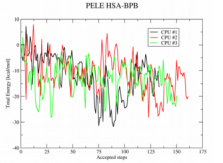
DPPC-EPB

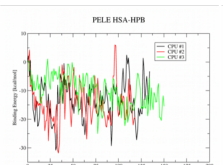
3) PELE's total and binding energy plots:

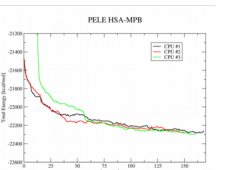


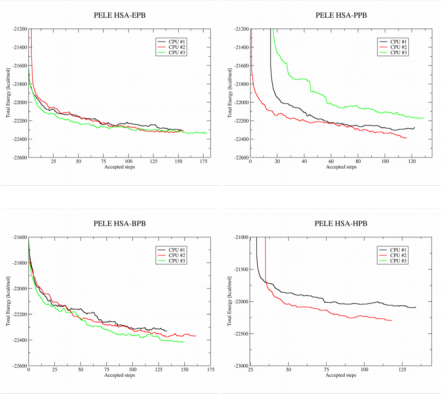












4) PELE's model input file:

```
energy params solvent vdgbnp
energy params ionic 0.1

## DO NOT CHANGE THE PDB FILE NAME IN THE FOLLOWING LINE
load pdb 5948.pdb ions no waters no het yes

#

pele &
     het B:583 &
     pdbmodel yes &
     init_min no &
     steered 1 &
     waitfor 2 &
     task &
          show bind_ene 1 &
          show rmsd_lig 1 heavy 0 &
          if random 1 gt 0.5 then rot_r 0.30 else rot_r 0.1 endif &
          if random 2 gt 0.5 then tra_r 6.0 tries 100 steric_tr 25
else tra_r 0.75 tries 5 steric_tr 250 endif &
```

```
     exit steps gt 400 &
end_task &
lcom_con 0.1 &
anmfreq 1 &
spfreq 1 &
mifreq 1 &
wrfreq 1 &
temp 2000 &
sprad 5.0 &
side &
     randomize no &
     verbose no &
     failsafe no &
     sideend &
path traj_ &
min &
     rmsg 0.04 &
     nbup yes &
     gbup yes &
     alphaup yes &
minimend &
caconst 0.5 &
rem_bulk_mov 3 &
anm_eig_freq 100000 &
anm_altm_freq 6 &
anm_altm_type 3 &
lanmanm neig 6  &
lanmanm move_ca 0.75 &
lanmanm mix_modes 0.75 &
lanmmin &
     mxitn 100 &
     iter 1 &
     rmsg 0.04 &
     nbup yes &
     alphaup no &
minimend
```